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Batch process monitoring based on functional data analysis and support vector data description

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ABSTRACT

Since the batch dataset is often organized as a special three-way array, i.e. (batches × variables × time), the research of data-based batch process monitoring has attracted much attention. This paper introduces a novel batch process monitoring framework based on functional data description (FDD), which treats each variable's trajectory varying with time in a batch process as a typical functional datum. Thus, the original batch process data can be transformed into a two-way manner (batches × functions of the variable trajectories) by describing each variable trajectory as a function. The FDD-based batch process monitoring method not only is effective to distinguish the subtle differences in the shape of variables' trajectories between normal batches and faulty batches, but also can easily handle some off-line data preprocessing steps, such as recovery of the missing data and trajectory alignment. Based on FDD, this paper extends a one-class classification method called support vector data description (SVDD) to its functional counterpart, which is called functional SVDD (FSVDD), and further proposes the algorithm of FSVDD-based batch process monitoring. Finally, two case studies, including a simulation example and an industrial semiconductor etch process, are used to illustrate the validity of the proposed FSVDD-based batch process monitoring method.

1. Introduction

Batch processes have been widely used in the chemical, pharmaceutical, biochemical, and semiconductor industries, due to the flexibility in the production. Process monitoring of batch processes is extremely important to ensure high quality products and safe operation, which has attracted many researchers' attention. Among all process monitoring methods, the data-based statistical process monitoring method has become one of the most important research topics.

Since the batch process data have the three-way structure, i.e. (batches × variables × time), traditional multivariable statistical process monitoring methods have to be adapted to batch processes. For instance, multiway principal component analysis (MPCA) [1,2], multiway partial least square (MPLS) [3] and multiway independent component analysis (MICA) [4] have already been proposed and widely used. After that, many variations of these methods have also been developed, such as hierarchical PCA [5], dynamic PCA and dynamic PLS for on-line batch process monitoring [6,7], sub-PCA modeling and monitoring strategy [8], and local and global PCA [9]. Besides, many actual batch processes often have the typical multi-stage/multi-phase characteristic. A batch process may have multiple processing units (called multi-stage), and/or a single processing unit may have multiple operational regimes (called multi-phase) [10–12]. In order to overcome these problems, different ways of phase segmentation and modeling methods have been developed. Yao and Gao [12] gave an detailed overview of the multi-stage/multi-phase batch process monitoring methods, including batch data preprocessing, phase division, and batch process modeling methods. Some recent works can be found in Yu and Qin [13], Sun et al. [14], Zhao et al. [15], Ge et al. [16], etc.

However, the existing nonlinear correlations between different variables in batch processes may extremely influence the linear monitoring methods' performance. Hence, the kernel trick has been introduced and the kernel counterparts of those batch process monitoring methods have also been developed, such as multiway kernel PCA [17], multiway kernel ICA [18], and hierarchical kernel PLS [19]. Essentially, the goal of batch process monitoring is to learn from abundant normal samples to build a model or an evaluation criterion, which is further used to detect unknown faults in the production process [20,21]. This can be considered as a typical one-class classification problem. Thus some pattern classification based monitoring methods have already been introduced, such as

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k-Nearest Neighbor (k-NN) [22], Gaussian Mixture Models (GMM) [13], and Hidden Markov Models (HMM) [23].

Besides, support vector machine (SVM) based monitoring approaches, such as one-class support vector machine (OCSVM) [24] and support vector data description (SVDD) [25], have received much attention recently. For example, Mahadevan and Shah [26] meticulously studied the fault detection performance of OCSVM in both the Tennessee Eastman process and a semiconductor etch process. Based on the SVDD model, several kinds of control charts have been proposed for multivariate process monitoring, such as K charts [27], robust K charts [28], and D^2 charts [29]. Furthermore, The SVDD method has also been combined with ICA for monitoring multivariate non-Gaussian processes [30–32]. Liu et al. [33] used the SVDD approach to improve the monitoring performance of nonlinear PCA and proposed the NPCA-SVDD monitoring scheme. Ge et al. [34] applied the SVDD approach to the batch process monitoring, and Ge and Song [35] further improved the batch process monitoring performance of the SVDD model by utilizing the bagging approach. Some more discussions about the recent developments of data-based process monitoring methods could be found in [36]. Compared with traditional PCA/PLS based process monitoring methods, OCSVM and SVDD have the following characteristics: (a) they can easily handle non-Gaussian, nonlinear, and/or multimodal data; (b) their fault detection models are only connected with a small part of the training data (called support vectors) directly, which makes the fault detection steps more convenient.

The basic idea of the conventional batch process monitoring methods mentioned above is to transform the three-way array into a two-way data matrix. The batch-wise unfolding method [1,2,37] and the variable-wise unfolding method [38] are the most commonly used approaches. However, these three-way data processing methods still have some shortcomings, such as the batch-wise unfolding method needs to synchronize trajectories and to equalize the batch lengths (see Section 2 for more details), and the variable-wise unfolding method couldn't remove the nonlinear dynamic effect from the process data since the unfolded matrix is centered just by subtracting a constant (i.e. the grand mean of each variable over all batches and all sampling times) from each variable trajectory in each batch [39]. Inspired by the functional data analysis (FDA) theory [40], this paper proposes a novel three-way array processing approach from the perspective of functional data. As the name implies, the FDA theory is to analysis the particular data which often show obvious functional features, such as the dynamic variation characteristics and the trend of fluctuations. The basic ideas of FDA were elaborated in the monograph by Ramsay and Silverman [40], and later some other monographs [41–44] further extended the research of the FDA theory and its applications. In conclusion, the FDA theory has been widely developed and widely used in many research fields, including statistics, economics, chemometrics, bioinformatics, geophysics, etc. Besides, the FDA method has already been introduced in some statistical monitoring problems, although the related works are very rare to the best of our knowledge. For example, Torres et al. [45] detected outliers in gas emissions by using FDA and the concept of functional depth. In profile monitoring, Yu et al. [46] used functional PCA to decompose the functional observations into the orthogonal function subspace, and detected outliers by defining the appropriate test statistic. These motivate us to consider the batch process data in another viewpoint.

Observing the collected three-way array in a batch process, one could find that the trajectories of some process variables often could be considered as sampled functions rather than just vectors and the dynamic time-varying features in the variable trajectories often show obvious functional nature, so these variables' trajectories often could be considered as the typical functional data. These characteristics motivate us to use the FDA theory to deal with some batch process monitoring problems. Hence, in this paper, we not only concern the correlation between different variables, but also take into account the functional nature of each variable trajectory. For this reason, this paper introduces the FDA method [40] to describe each trajectory as an appropriate function, and constitutes a novel two-way manner (i.e. batches × functions of the variable trajectories) of the batch process data, which is called functional data description (FDD) in this paper.

As a consequence, the main contribution of this paper is to combine FDD and SVDD to monitor the batch processes. By using FDD to represent the batch process data and extending the SVDD method to its functional counterpart which is called functional SVDD (FSVDD), the FSVDD-based batch process monitoring method is proposed. The rest of this paper is organized as follows. Section 2 introduces how to transform the three-way array to FDD by using FDA. After a brief introduction to the conventional SVDD model, the principle of functional SVDD is discussed in Section 3. Section 4 introduces the FSVDD-based batch process monitoring method in detail. In order to evaluate the performance of the proposed FSVDD-based monitoring method, two case studies including a simulation example and an industrial semiconductor etch process are provided in Section 5. Finally, some conclusions are made in Section 6.

2. Representing three-way array by functional data analysis

2.1. Conventional methods

In most literature, batch process data are often organized as a three-way array $\underline{X}(I \times J \times K)$ (Fig. 1a), where I is the number of batches, J is the number of variables, and K is the number of sampling times in a given batch. An observation of variable j ($j = 1, \ldots, J$) at sampling time k ($k = 1, \ldots, K$) in batch run i ($i = 1, \ldots, I$) is denoted as $x_{i,j,k}$. Here, it assumes that each batch has the same length K, which is not often satisfied in actual problems. In fact, in most industrial processes, different batches may have different sampling intervals and/or different sampling durations. So more precisely, the vector of variable j in batch run i should be denoted as $\mathbf{x}_{i,j} = [x_{i,j,1}, \ldots, x_{i,j,K_i}]^T$, where the number of sampling times K_i depends on the batch index i. However, many traditional batch process monitoring methods, such as MPCA and MPLS, require that the training dataset should have the regular three-way structure. Hence, in order to obtain the three-way array $\underline{X}(I \times J \times K)$, some data preprocessing steps, such as trajectory alignment/synchronization and batch length equalization, are often needed. For example, dynamic time warping (DTW) [47] or correlation optimized warping (COW) [48] is often used to equalize the batch lengths.

At present, the widely used batch process monitoring methods are based on the three-way data unfolding approaches, which unfold the three-way array $\underline{X}$ to a two-way data matrix $\mathbf{X}$. The structure of the two-way matrix is based on the particular monitoring problems and particular applications. There is a summary about data unfolding approaches in [49]. It shows that there are totally K different kinds of unfolding forms, which can all be denoted as $\mathbf{X}((K - a + 1)I \times aJ)$, where $a = 1, 2, \ldots, K$ [49]. Among them, the data unfolding form with $a = 1$ and $a = K$ are the most famous ones. When $a = 1$ (also called the variable-wise unfolding method [38]), the corresponding two-way matrix $\mathbf{X}(KI \times J)$ is shown in the right side of Fig. 1a (It should be noted that, in fact, the variable-wise unfolding method often does not need the data preprocessing steps, such as trajectory alignment or batch length equalization). When $a = K$ (also called the batch-wise unfolding method [1,2,37]), the corresponding two-way matrix $\mathbf{X}(I \times KJ)$ is shown in the bottom of Fig. 1a. The former is often used in the real-time online batch process monitoring, while the latter is often used in the end-of-batch